# Nonparametric and Semi-Parametric Goodness of Fit

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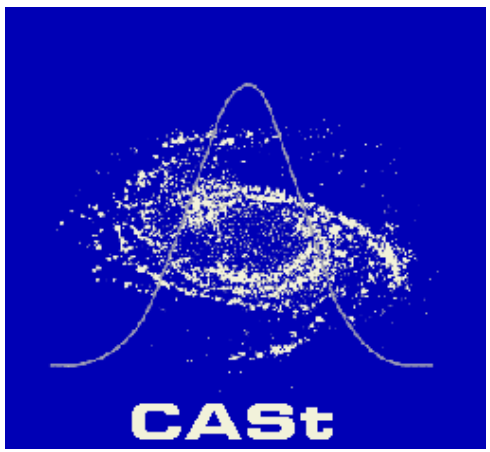



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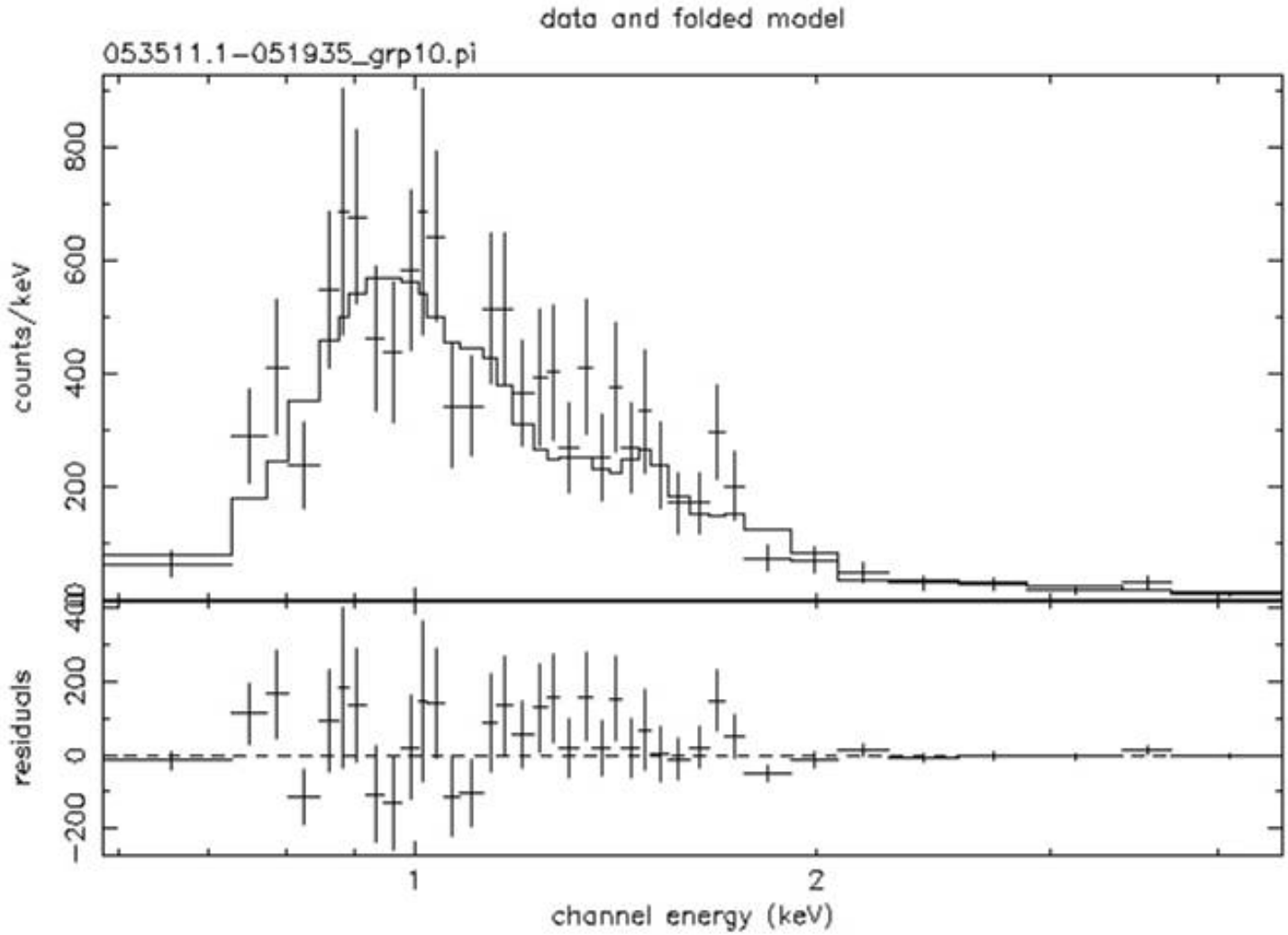
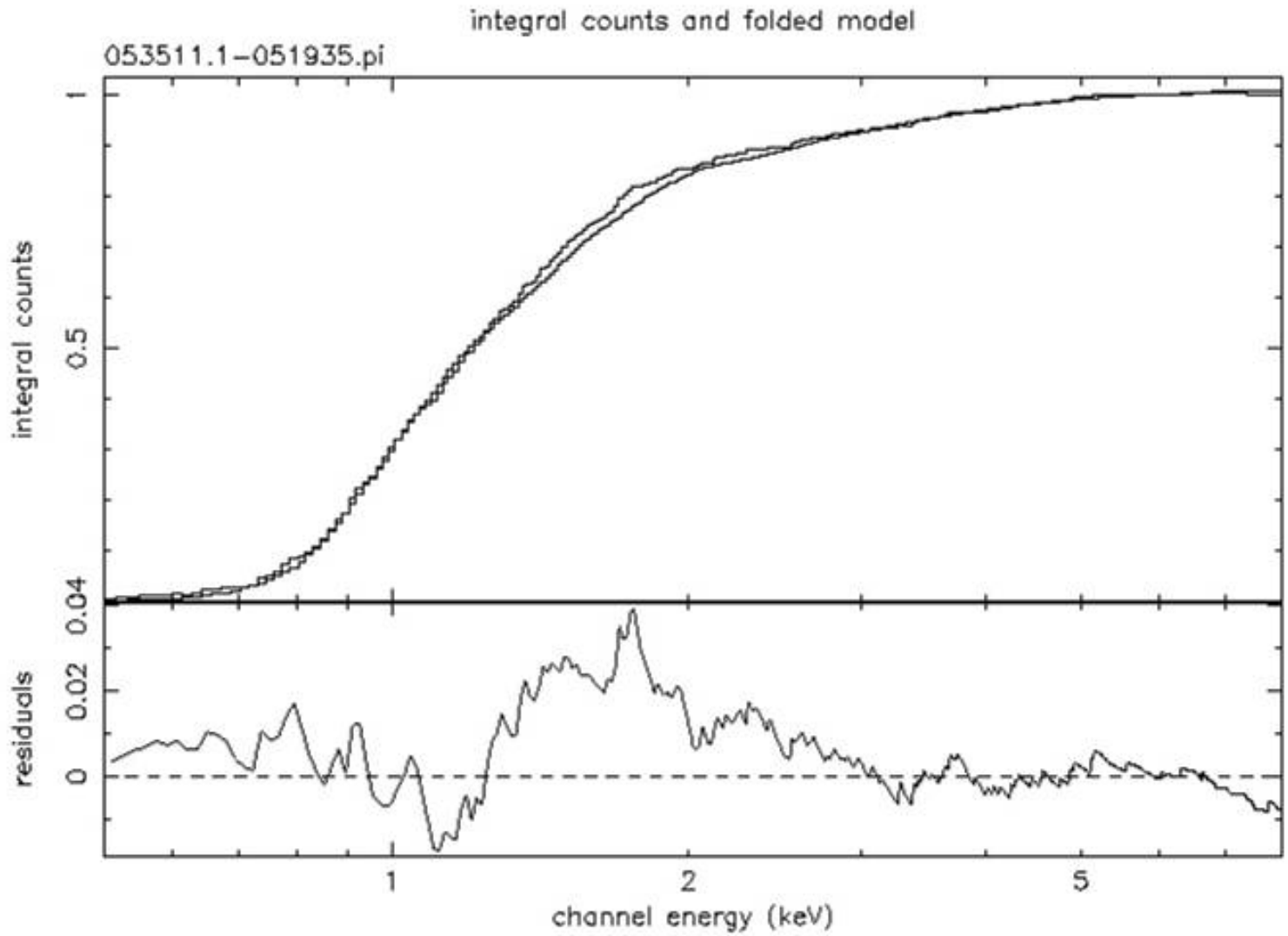
# Astrophysical Inference from astronomical data

## Fitting astronomical data

- Non-linear regression
- Density (shape) estimation
- Parametric modeling
  - Parameter estimation of assumed model
  - Model selection to evaluate different models
    - Nested (in quasar spectrum, should one add a broad absorption line BAL component to a power law continuum)
    - Non-nested (is the quasar emission process a mixture of blackbodies or a power law?)
- Goodness of fit

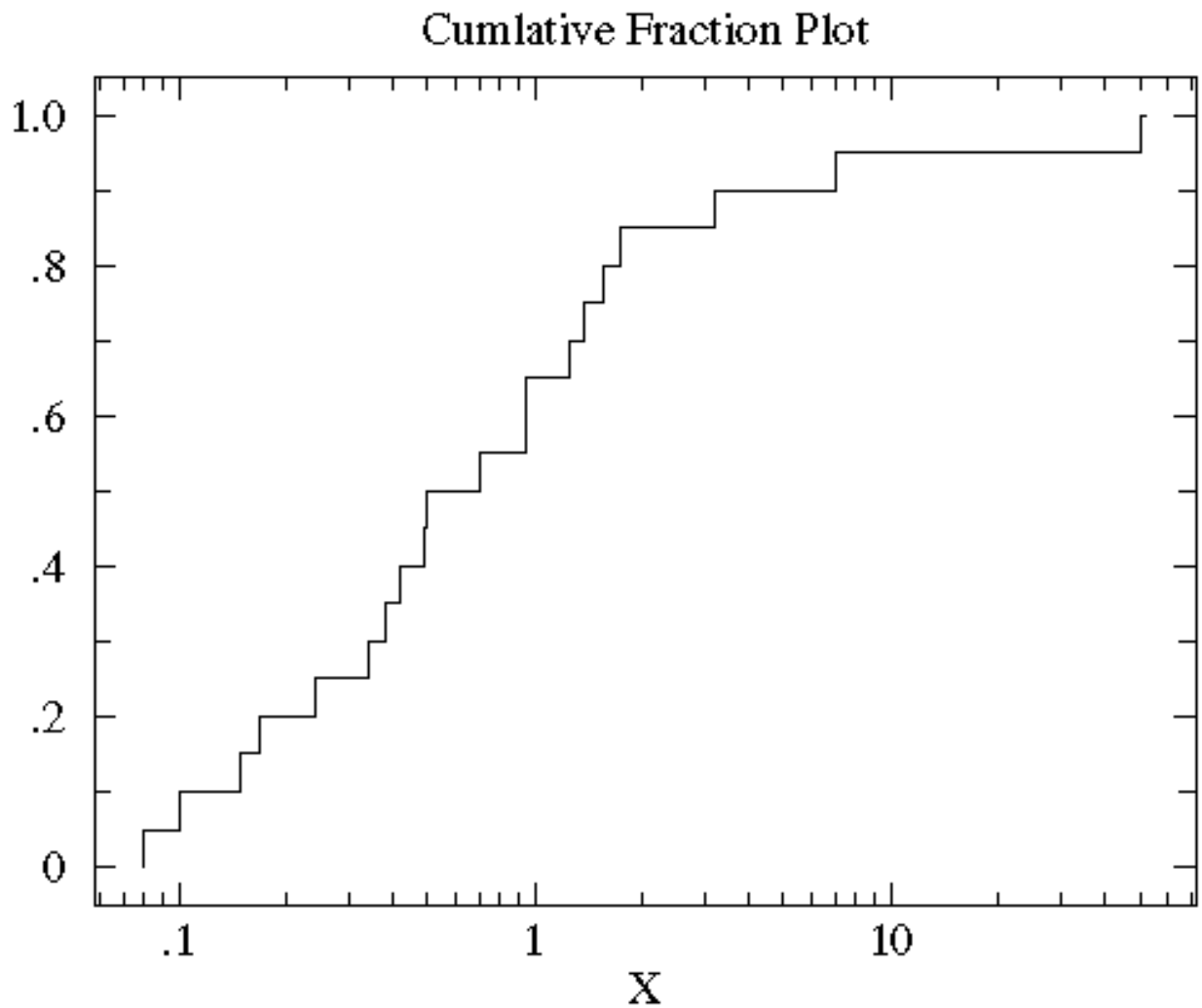


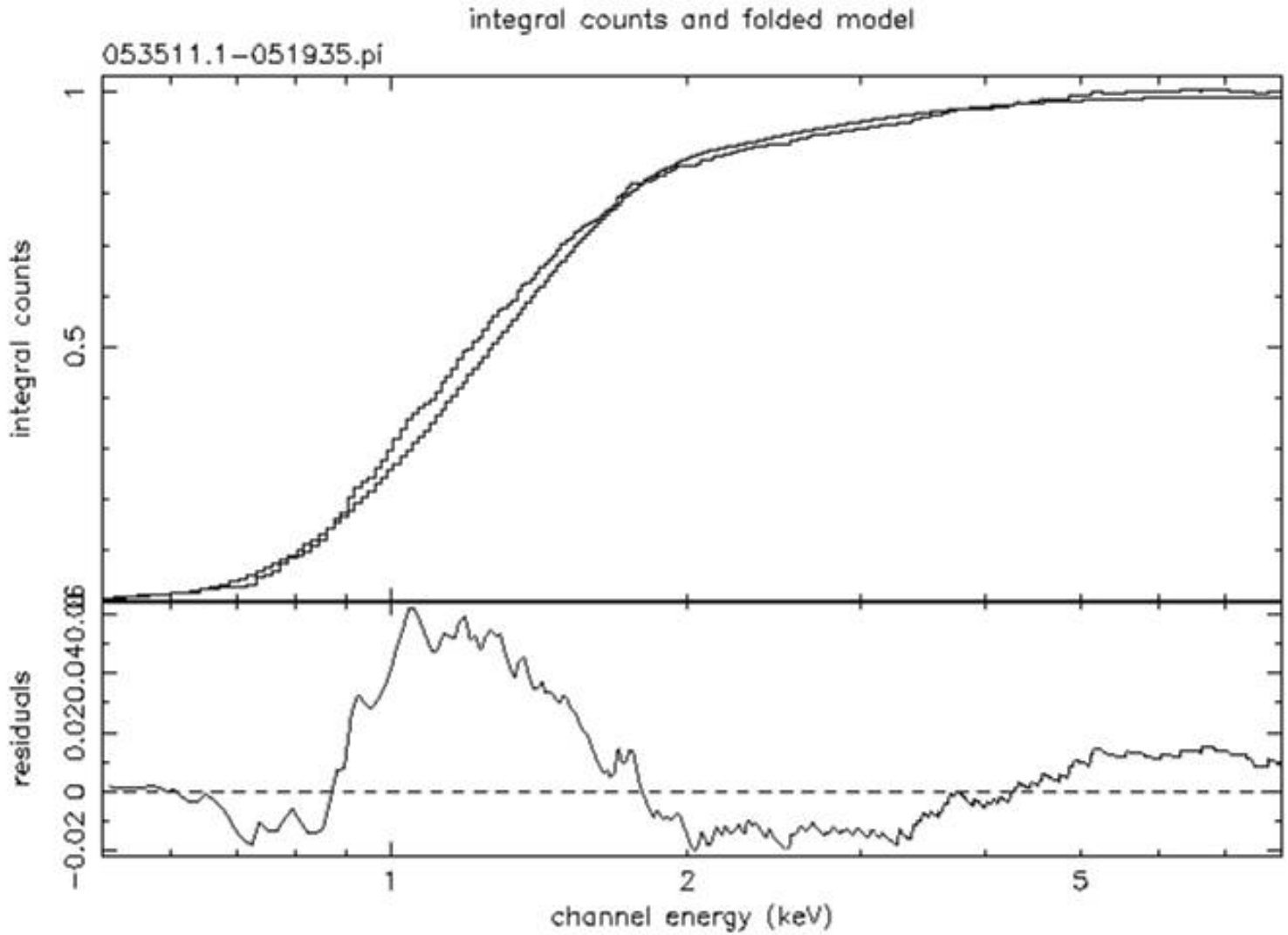

**Chandra X-ray Observatory ACIS data**
**COUP source # 410 in Orion Nebula with 468 photons**
**Fitting to binned data using $\chi^2$ (XSPEC package)**
**Thermal model with absorption, $A_V$~1 mag**




**Fitting to unbinned EDF**
**Maximum likelihood (C-statistic)**
**Thermal model with absorption**

# Empirical Distribution Function





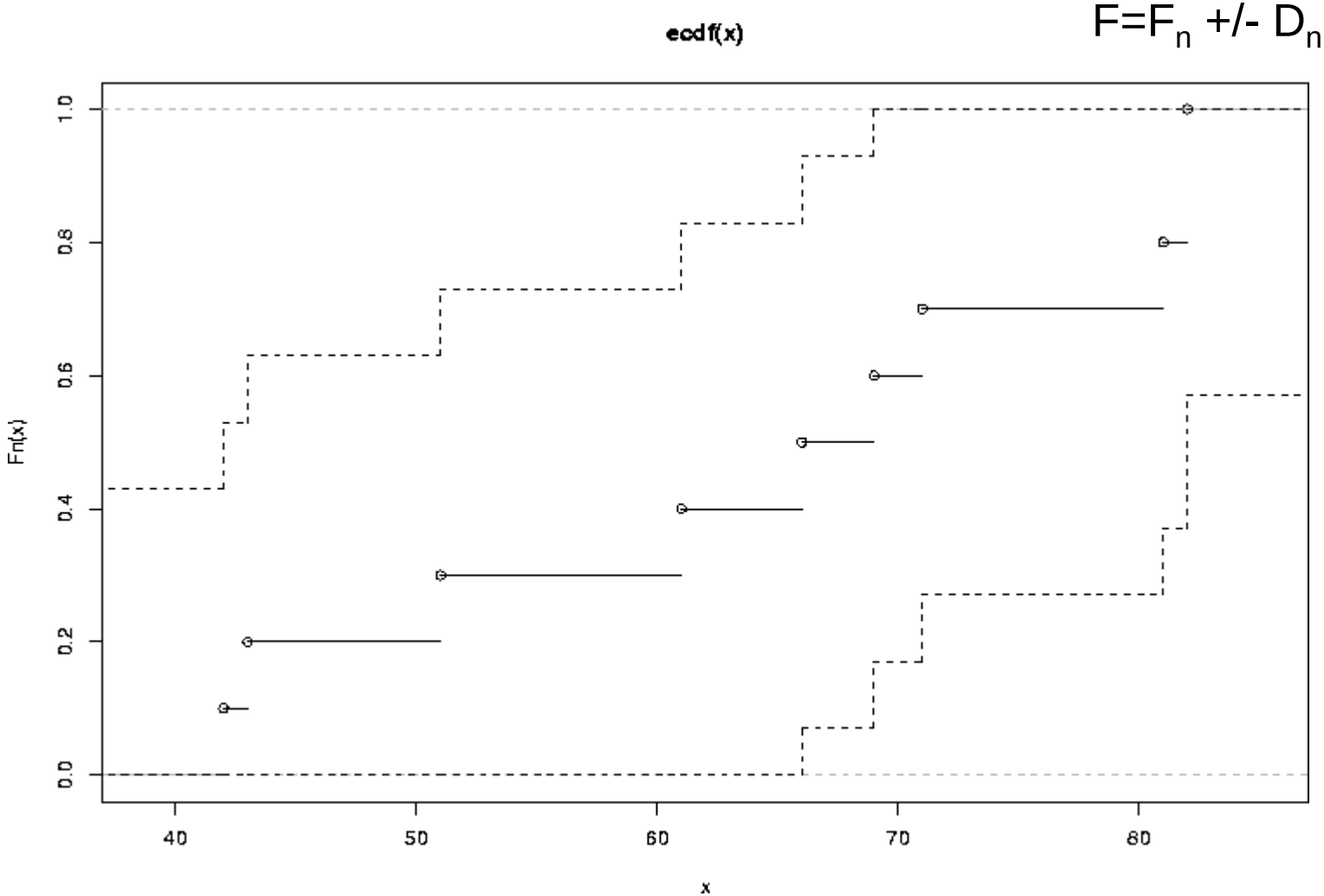

**Incorrect model family**

**Power law model, absorption $A_V$~1 mag**

**Question : Can a power law model be excluded with 99% confidence?**

# K-S Confidence bands

$F=F_n$ +/- $D_n(\alpha)$



# Model fitting

Aim: To provide most parsimonious `best' fit

To answer:

- Is the underlying nature of a stellar spectrum a non-thermal power law or a thermal gas with absorption?
- Are the fluctuations in the cosmic microwave background best fit by Big Bang models with dark energy or with quintessence?
- Are there interesting correlations among the properties of objects in any given class (e.g. the Fundamental Plane of elliptical galaxies), and what are the optimal analytical expressions of such correlations?

# Statistics Based on EDF

**Kolmogrov-Smirnov:** $\text{Sup}_x |F_n(x) - F(x)|$,

$\text{Sup}_x (F_n(x) - F(x))^+$, $\text{Sup}_x (F_n(x) - F(x))^-$

**Cramer - van Mises:** $\int (F_n(x) - F(x))^2 \, dF(x)$

**Anderson - Darling:** $\int \frac{(F_n(x) - F(x))^2}{F(x)(1 - F(x))} \, dF(x)$

All of these statistics are distribution free

**Nonparametric statistics**

**Table 1. Limiting Distribution of the Kolmogorov-Smirnov Statistic**
(from Smirnov (1948))

| $x$ | $L(x)$ | $x$ | $L(x)$ | $x$ | $L(x)$ | $x$ | $L(x)$ |
|---|---|---|---|---|---|---|---|
| 0.28 | 0.000001 | 0.73 | 0.339113 | 1.18 | 0.876548 | 1.76 | 0.995922 |
| 0.29 | 0.000004 | 0.74 | 0.355981 | 1.19 | 0.882258 | 1.78 | 0.996460 |
| 0.30 | 0.000009 | 0.75 | 0.372833 | 1.20 | 0.887750 | 1.80 | 0.996932 |
| 0.31 | 0.000021 | 0.76 | 0.389640 | 1.21 | 0.893030 | 1.82 | 0.997346 |
| 0.32 | 0.000046 | 0.77 | 0.406372 | 1.22 | 0.898104 | 1.84 | 0.997707 |
| 0.33 | 0.000091 | 0.78 | 0.423002 | 1.23 | 0.902972 | 1.86 | 0.998023 |
| 0.34 | 0.000171 | 0.79 | 0.439505 | 1.24 | 0.907648 | 1.88 | 0.998297 |
| 0.35 | 0.000303 | 0.80 | 0.455857 | 1.25 | 0.912132 | 1.90 | 0.998536 |
| 0.36 | 0.000511 | 0.81 | 0.472041 | 1.26 | 0.916432 | 1.92 | 0.998744 |
| 0.37 | 0.000826 | 0.82 | 0.488030 | 1.27 | 0.920556 | 1.94 | 0.998924 |
| 0.38 | 0.001285 | 0.83 | 0.503808 | 1.28 | 0.924505 | 1.96 | 0.999079 |
| 0.39 | 0.001929 | 0.84 | 0.519366 | 1.29 | 0.928288 | 1.98 | 0.999213 |
| 0.40 | 0.002808 | 0.85 | 0.534682 | 1.30 | 0.931908 | 2.00 | 0.999329 |
| 0.41 | 0.003972 | 0.86 | 0.549744 | 1.31 | 0.935370 | 2.02 | 0.999428 |
| 0.42 | 0.005476 | 0.87 | 0.564546 | 1.32 | 0.938682 | 2.04 | 0.999516 |
| 0.43 | 0.007377 | 0.88 | 0.579070 | 1.33 | 0.941848 | 2.06 | 0.999588 |
| 0.44 | 0.009730 | 0.89 | 0.593316 | 1.34 | 0.944872 | 2.08 | 0.999650 |
| 0.45 | 0.012590 | 0.90 | 0.607270 | 1.35 | 0.947756 | 2.10 | 0.999705 |
| 0.46 | 0.016005 | 0.91 | 0.620928 | 1.36 | 0.950512 | 2.12 | 0.999750 |
| 0.47 | 0.020022 | 0.92 | 0.634286 | 1.37 | 0.953142 | 2.14 | 0.999790 |
| 0.48 | 0.024682 | 0.93 | 0.647338 | 1.38 | 0.955650 | 2.16 | 0.999822 |
| 0.49 | 0.030017 | 0.94 | 0.660082 | 1.39 | 0.958040 | 2.18 | 0.999852 |
| 0.50 | 0.036055 | 0.95 | 0.672516 | 1.40 | 0.960318 | 2.20 | 0.999874 |
| 0.51 | 0.042814 | 0.96 | 0.684636 | 1.41 | 0.962486 | 2.22 | 0.999896 |
| 0.52 | 0.050306 | 0.97 | 0.696444 | 1.42 | 0.964552 | 2.24 | 0.999912 |
| 0.53 | 0.058534 | 0.98 | 0.707940 | 1.43 | 0.966516 | 2.26 | 0.999926 |
| 0.54 | 0.067497 | 0.99 | 0.719126 | 1.44 | 0.968382 | 2.28 | 0.999940 |
| 0.55 | 0.077183 | 1.00 | 0.730000 | 1.45 | 0.970158 | 2.30 | 0.999949 |
| 0.56 | 0.087577 | 1.01 | 0.740566 | 1.46 | 0.971846 | 2.32 | 0.999958 |
| 0.57 | 0.098656 | 1.02 | 0.750826 | 1.47 | 0.973448 | 2.34 | 0.999965 |
| 0.58 | 0.110395 | 1.03 | 0.760780 | 1.48 | 0.974970 | 2.36 | 0.999970 |
| 0.58 | 0.122760 | 1.04 | 0.770434 | 1.49 | 0.976412 | 2.38 | 0.999976 |
| 0.60 | 0.135718 | 1.05 | 0.779794 | 1.50 | 0.977782 | 2.40 | 0.999980 |
| 0.61 | 0.149229 | 1.06 | 0.788860 | 1.52 | 0.980310 | 2.42 | 0.999984 |
| 0.62 | 0.163225 | 1.07 | 0.797636 | 1.54 | 0.982578 | 2.44 | 0.999987 |
| 0.63 | 0.177753 | 1.08 | 0.806128 | 1.56 | 0.984610 | 2.46 | 0.999989 |
| 0.64 | 0.192677 | 1.09 | 0.814342 | 1.58 | 0.986426 | 2.48 | 0.999991 |
| 0.65 | 0.207987 | 1.10 | 0.822282 | 1.60 | 0.988048 | 2.58 | 0.999 9925 |
| 0.66 | 0.223637 | 1.11 | 0.829950 | 1.62 | 0.989492 | 2.55 | 0.999 9956 |
| 0.67 | 0.239582 | 1.12 | 0.837356 | 1.64 | 0.990777 | 2.60 | 0.999 9974 |
| 0.68 | 0.255780 | 1.13 | 0.844502 | 1.66 | 0.991917 | 2.65 | 0.999 9984 |
| 0.69 | 0.272189 | 1.14 | 0.851394 | 1.68 | 0.992928 | 2.70 | 0.999 9990 |
| 0.70 | 0.288765 | 1.15 | 0.858038 | 1.70 | 0.993823 | 2.80 | 0.999 9997 |
| 0.71 | 0.305471 | 1.16 | 0.864442 | 1.72 | 0.994612 | 2.90 | 0.999 99990 |
| 0.72 | 0.322265 | 1.17 | 0.870612 | 1.74 | 0.995309 | 3.00 | 0.999 99997 |

KS Probabilities are invalid under common astronomical usage.

(Lillifors 1964)

# Statistics Based on EDF

**Kolmogrov-Smirnov:** $\text{Sup}_x |F_n(x) - F(x)|$

**Cramer - van Mises:** $$\int (F_n(x) - F(x))^2 \, dF(x)$$

**Anderson - Darling:** $$\int \frac{(F_n(x) - F(x))^2}{F(x)(1 - F(x))} \, dF(x)$$

All of these statistics are no longer distribution free if parameters are estimated or the data is multivariate.

# Multivariate Case

**Warning:** K-S does not work in multidimensions

**Example – Paul B. Simpson (1951)**

$F(x,y) = ax^2 y + (1 - a) y^2 x, \quad 0 < x, y < 1$

$(X_1, Y_1)$ data from F, $F_1$ EDF of $(X_1, Y_1)$

$P(|F_1(x,y) - F(x,y)| < 0.72$, for all x, y) **is**

$> 0.065$ if $a = 0$, $(F(x,y) = y^2 x)$

$< 0.058$ if $a = 0.5$, $(F(x,y) = xy(x+y)/2)$

Numerical Recipe's treatment of a 2-dim KS test is mathematically invalid.

# Processes with estimated Parameters

$\{F(.; \theta): \theta \in \Theta\}$ - a family of distributions

$X_1, \ldots, X_n$ sample from F

Kolmogorov-Smirnov, Cramer-von Mises etc., when $\theta$ is estimated from the data, are Continuous functionals of the empirical process

$$Y_n(x; \theta_n) = \sqrt{n}\,(F_n(x) - F(x; \theta_n))$$

In the Gaussian case,

$\theta = (\mu,\sigma^2)$ and $\theta_n = (\overline{X}, s_n^2)$

$$\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

$$s_n^2 = \frac{1}{n}\sum_{i=1}^{n} (X_i - \overline{X})^2$$

# Bootstrap

$\hat{F}_n$ is an estimator of $F$, based $X_1, \ldots, X_n$.

$X_1^*, \ldots, X_n^*$ i.i.d. from $\hat{F}_n$

$\hat{\theta}_n^* = \theta_n(X_1^*, \ldots, X_n^*)$

$F(.;\theta)$ is Gaussian with $\theta = (\mu, \sigma^2)$

If $\hat{\theta}_n = (\bar{X}_n, s_n^2)$, then

$\hat{\theta}_n^* = (\bar{X}_n^*, s_n^{*2})$

Parametric bootstrap if $\hat{F}_n = F(.;\hat{\theta}_n)$

$X_1^*, \ldots, X_n^*$ i.i.d. $F(.;\mu,\sigma^2)$

Nonparametric bootstrap if $\hat{F}_n = F_n$

# Parametric Bootstrap

$X_1^*, \ldots, X_n^*$ sample generated from $F(.; \theta_n)$.

In Gaussian case $\theta_n^* = (\overline{X}_n^*, s_n^{*2})$.

Both $\sqrt{n}\, \sup_x |F_n(x) - F(x; \theta_n)|$ and

$\sqrt{n}\, \sup_x |F_n^*(x) - F(x; \theta_n^*)|$

have the same limiting distribution

(In the XSPEC packages, the parametric bootstrap is command FAKEIT, which makes Monte Carlo simulation of specified spectral model)

# Nonparametric Bootstrap

$X_1^*, \ldots, X_n^*$ *i.i.d.* from $F_n$.

A bias correction

$B_n(x) = F_n(x) - F(x; \theta_n)$

is needed.

$\sqrt{n}\ \sup_x |F_n(x) - F(x; \theta_n)|$ and

$\sqrt{n}\ \sup_x |F_n^*(x) - F(x; \theta_n^*) - B_n(x)|$

have the same limiting distribution

(XSPEC does not provide a nonparametric bootstrap capability)

- **Chi-Square type statistics** – (Babu, 1984, Statistics with linear combinations of chi-squares as weak limit. *Sankhya*, Series A, **46**, 85-93.)

- **U-statistics** – (Arcones and Giné, 1992, On the bootstrap of U and V statistics. *Ann. of Statist.*, **20**, 655–674.) Resampling methods for semi-parametricgoodness-of-fit tests – p. 12/28

# Confidence limits under misspecification of model family

$X_1, \ldots, X_n$ data from unknown H.

H may or may not belong to the family $\{F(.; \theta): \theta \in \Theta\}$.

H is closest to $F(.; \theta_0)$, in Kullback - Leibler information

$$\int h(x) \log (h(x)/f(x; \theta)) \, d\nu(x) \geq 0$$

$$\int h(x) |\log (h(x)| \, d\nu(x) < \infty$$

$$\int h(x) \log f(x; \theta_0) \, d\nu(x) = \max_\theta \int h(x) \log f(x; \theta) \, d\nu(x)$$

For any $0 < \alpha < 1$,

$$P(\sqrt{n}\ \sup_x |F_n(x) - F(x; \theta_n) - (H(x) - F(x; \theta_0))| < C_\alpha^*) \rightarrow \alpha$$

$c_\alpha^*$ is the $\alpha$-th quantile of

$$\sqrt{n}\ \sup_x |F_n^*(x) - F(x; \theta_n^*) - (F_n(x) - F(x; \theta_n))|$$

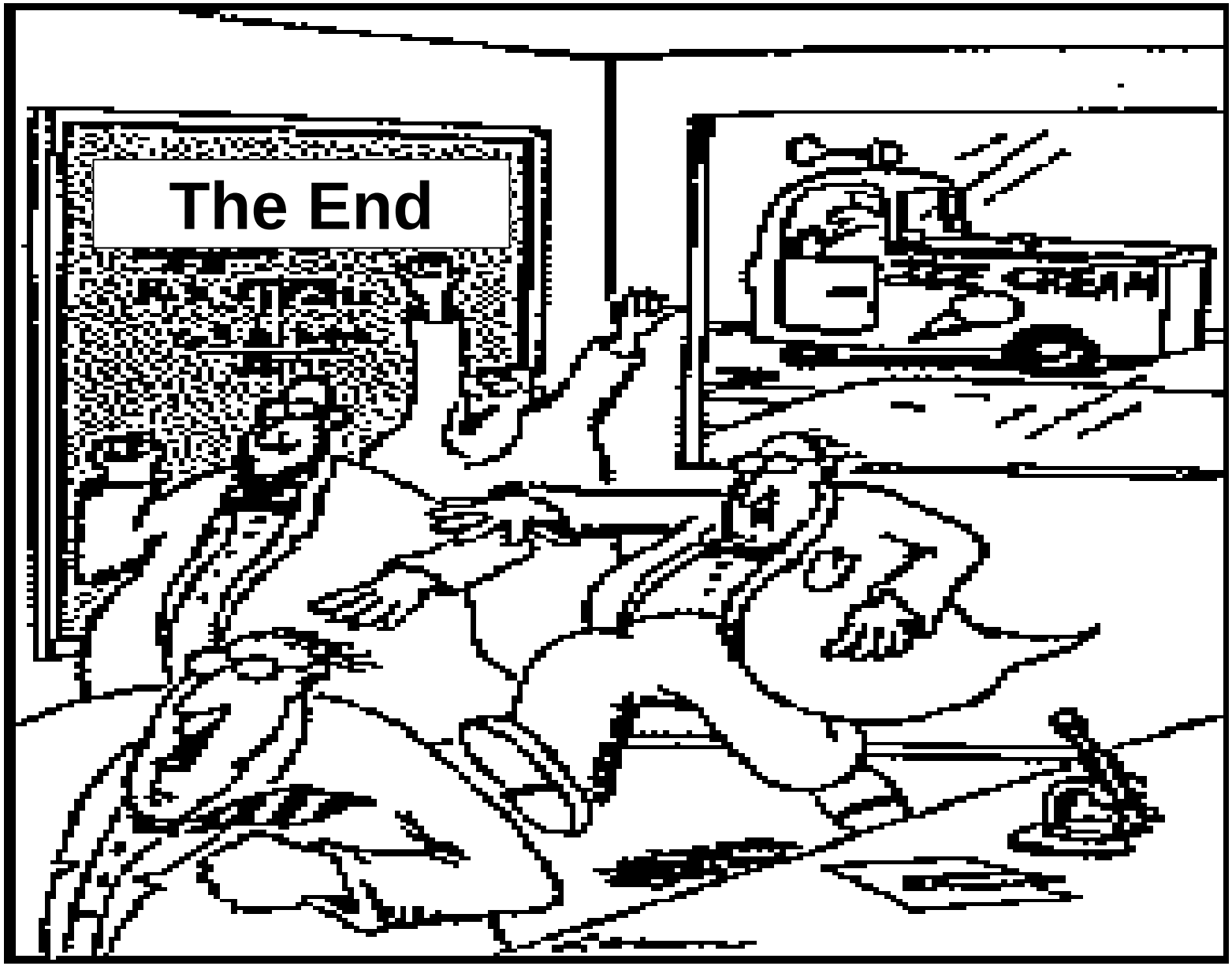
This provide an estimate of the distance between the true distribution and the family of distributions under consideration.

# References


- **Bootstrap Methodology**
  - G. J. Babu and C. R. Rao (1993). Handbook of Statistics, Vol 9, Chapter 19.
  - G. J. Babu and C. R. Rao (2003). Confidence limits to the distance of the true distribution from a misspecified family by bootstrap. *J. Statist. Plann. Inference* **115**, 471-478.

- **Bootstrap Techniques for Signal Processing**
  Abdelhak M. Zoubir and D. Robert Iskander, Cambridge, U.K.: Cambridge University Press, 2004.

  This book serves as a handbook on *bootstrap* for engineers, to analyze complicated data with little or no model assumptions. Bootstrap has found many applications in engineering field including, artificial neural networks, biomedical engineering, environmental engineering, image processing, and Radar and sonar signal processing. Majority of the applications are taken from signal processing literature.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